Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
Welcome to STN International
NEWS
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
                 "Ask CAS" for self-help around the clock
NEWS
         Jul 12 BEILSTEIN enhanced with new display and select options,
                 resulting in a closer connection to BABS
         AUG 02
                 IFIPAT/IFIUDB/IFICDB reloaded with new search and display
NEWS
                 fields
         AUG 02
NEWS
     5
                 CAplus and CA patent records enhanced with European and Japan
                 Patent Office Classifications
                 The Analysis Edition of STN Express with Discover!
NEWS
         AUG 02
                 (Version 7.01 for Windows) now available
NEWS
     7
         AUG 27
                 BIOCOMMERCE: Changes and enhancements to content coverage
NEWS
         AUG 27
                 BIOTECHABS/BIOTECHDS: Two new display fields added for legal
                 status data from INPADOC
NEWS 9
         SEP 01
                 INPADOC: New family current-awareness alert (SDI) available
NEWS 10
         SEP 01
                 New pricing for the Save Answers for SciFinder Wizard within
                 STN Express with Discover!
                 New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
NEWS 11
         SEP 01
NEWS 12 SEP 14
                STN Patent Forum to be held October 13, 2004, in Iselin, NJ
NEWS 13 SEP 27
                 STANDARDS will no longer be available on STN
                 SWETSCAN will no longer be available on STN
NEWS 14 SEP 27
NEWS 15 SEP 30 STN downtime scheduled October 2-3, 2004
NEWS EXPRESS JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS
              STN Operating Hours Plus Help Desk Availability
NEWS INTER
              General Internet Information
NEWS LOGIN
              Welcome Banner and News Items
NEWS PHONE
              Direct Dial and Telecommunication Network Access to STN
NEWS WWW
              CAS World Wide Web Site (general information)
```

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 12:21:11 ON 05 OCT 2004

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FILE 'REGISTRY' ENTERED AT 12:21:23 ON 05 OCT 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 OCT 2004 HIGHEST RN 756793-93-8 DICTIONARY FILE UPDATES: 4 OCT 2004 HIGHEST RN 756793-93-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> logoff hold COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.42 0.63

FULL ESTIMATED COST

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 12:21:30 ON 05 OCT 2004

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD.

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * * SESSION RESUMED IN FILE 'REGISTRY' AT 12:24:20 ON 05 OCT 2004 FILE 'REGISTRY' ENTERED AT 12:24:20 ON 05 OCT 2004 COPYRIGHT (C) 2004 American Chemical Society (ACS)

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

0.42 0.63

=>

Uploading C:\Examination Auxillary files\10796093\10796093 clmd cmpd.str

chain nodes:
7 8 9 10 11 12 13 14

ring nodes:
1 2 3 4 5 6

chain bonds:
2-11 3-12 5-7 7-8 8-9 9-10 11-13 12-14

ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds:
2-11 3-12 9-10 11-13

exact bonds:
5-7 7-8 8-9 12-14

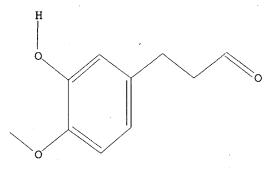
normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 11 exact full FULL SEARCH INITIATED 12:25:34 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 146 TO ITERATE

100.0% PROCESSED 146 ITERATIONS SEARCH TIME: 00.00.01

1 ANSWERS

L2 1 SEA EXA FUL L1

=> d scan

L2 1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN IN Benzenepropanal, 3-hydroxy-4-methoxy- (9CI)

MF C10 H12 O3

d.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> d 12

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 333754-84-0 REGISTRY

CN Benzenepropanal, 3-hydroxy-4-methoxy- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-(3-Hydroxy-4-methoxyphenyl)propionaldehyde

FS 3D CONCORD

MF C10 H12 O3

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 55.70 55.91

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 12:26:39 ON 05 OCT 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching

databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 5 Oct 2004 VOL 141 ISS 15 FILE LAST UPDATED: 4 Oct 2004 (20041004/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 12 L3 3 L2

=> d 13 1-3 ti fbib abs

L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

TI Process for producing cinnamyl aldehyde derivatives and use thereof as intermediate for aspartame derivative

AN 2001:851092 CAPLUS

DN 135:371997

TI Process for producing cinnamyl aldehyde derivatives and use thereof as intermediate for aspartame derivative

IN Mori, Kenichi; Fujita, Shinji; Funakoshi, Nao; Takemoto, Tadashi

PA Ajinomoto Co., Inc., Japan

SO PCT Int. Appl., 29 pp. CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

TIM.			NO.			KIND DATE				APPLICATION NO.						DATE			
ΡI	WO 2001087813				A1 20011122			ī	WO 2	001-	JP35	45							
		W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,	
			co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	
			HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	
			LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	ΝZ,	PL,	PT,	RO,	
			RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	
			VN,	YU,	ZA,	ZW,	AM,	ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM				
		RW:	GH,	GM,	ΚE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,	
			DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,	
			ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GW,	ML,	MR,	ΝE,	SN,	TD,	ΤG			
										1	JP 2	000-	1428	11	i	A 2	0000	516	
	EP	1283								EP 2001-922073				20010424					
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	ΝL,	SE,	MC,	PT,	
			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	ΑL,	TR							
											JP 2	000-	1428	11	i	A 2	0000	516	
										1	WO 2	001-	JP35	45	1	W 2	0010	424	
	US	2003	1630	04		A 1		2003	0828	1	US 2	002-	2959	97		2	0021	118	
											JP 2	000-	1428	11	2	A 2	0000	516	
										1	WO 2	001-	JP35	45	1	A1 2	0010	424	

CASREACT 135:371997; MARPAT 135:371997

OS GI

AB Described is an industrial process for conveniently and efficiently producing highly pure cinnamyl aldehyde derivs. (I; R = H, C1-4 alkyl or alkoxy) such as (2E)-(3-hydroxy-4-methoxy) cinnamyl aldehyde which comprises reacting a benzaldehyde derivative (II; R = same as above) (for example, isovanillin) with acetaldehyde in the presence of an alkali, preferably adding acetaldehyde in portions in an aqueous solution at a low temperature

The cinnamyl aldehyde derivs. (I) thus obtained are selectively reduced into 3-(3-hydroxy-4-substituted phenyl)propionaldehydes (III; R = same as above). These compds. III are further subjected to reductive alkylation with aspartame to efficiently give N-[N-[3-(3-hydroxy-4-substituted phenyl)propyl]-L-α-aspartyl]-L-phenylalanine 1-Me esters (IV; R = H, C1-4 alkyl or alkoxy), which are useful as sweeteners with high sweetness. Thus, 121.72 g isovanillin and 320 g NaOH were dissolved in 2,000 mL H2O and cooled to -10°, followed by continuously adding 290 g 28 weight% aqueous acetaldehyde over a period of 45 h, and the resulting mixture was stirred for 1 h, treated with 768.1 g 36 weight% aqueous HCl, and filtered to give 324 g crystalline product. The latter product was dispersed in 500 mL H2O at 25°, treated with 97.5 g 25 weight% aqueous NaOH for dissoln., stirred with 4 g activated charcoal and 16 g celite, and filtered. The filtrate was neutralized with 55.4 g 36 weight% aqueous HCl to give 185.5 g crystalline product

which was vacuum-dried, dispersed in 275 mL MeOH at 60° , stirred for 2 h, cooled to room temperature, and filtered to give, after drying the wet crystals, 83.2 g (2E)-3-hydroxy-4-methoxycinnamaldehyde (98% purity) in 57% yield. The latter compound (5.00 g) and 300 mg 5% Pd-Al2O3 were added to 80 mL MeOH and stirred under H atmospheric at 35° for 24 h, followed by filtration for removal of the catalyst and washing the catalyst with 10 mL MeOH, to give a MeOH solution of 3-(3-hydroxy-4-methoxyphenyl)propionaldehyde (87% yield). The latter solution (8.15 g) containing 1.50 g of the aldehyde

2.57 g aspartame were added to a 4:1 mixture of MeOH and H2O, followed by adding 0.7 g 10% Pd-C containing 50% H2O, and the resulting mixture was stirred at 35° under H atmospheric for 48 h to give 71% N-[N-[3-(3-hydroxy-4-methoxyphenyl)propyl]-L- α -aspartyl]-L-phenylalanine 1-Me ester.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
- TI N-Alkylaspartyl dipeptide esters and low-calorie sweeteners containing them
- AN 2001:842307 CAPLUS
- DN 135:370940

and

TI N-Alkylaspartyl dipeptide esters and low-calorie sweeteners containing them

IN Amino, Yusuke; Yuzawa, Kazuko

PA Ajinomoto Co., Inc., Japan

SO Jpn. Kokai Tokkyo Koho, 6 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
		-			
PI	JP 2001322996	A2	20011120	JP 2000-142808	20000516
				JP 2000-142808	20000516
	405 050040				

OS MARPAT 135:370940

GΙ

AB Sweeteners contain title compds. I (R1-R5 = H, OH, C1-3 alkoxy, C1-3 alkyl, C2-3 hydroxyalkyloxy; R6-R10 = H, C1-3 alkyl; R11 = C1-5 alkyl; R12 = H, C1-3 alkyl; R13 = C1-4 alkyl; X = O, S; n = 1, 2) or their salts. A THF solution of 967 mg α -L-aspartyl-(S-tert-butyl)-L-cysteine Me ester was condensed with 360 mg 3-(3-hydroxy-4-methoxyphenyl)propionaldehyde in the presence of AcOH and NaB(OAc)3H at room temperature overnight to give 596

Ι

mg I (R1 = R4-R10 = R12 = H, R2 = OH, R3 = OMe, R11 = CMe3, R13 = Me, X = S, n = 1), which was 40,000 times as sweet as sucrose.

L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

Process for the production of aspartyldipeptide ester derivatives, novel intermediates therefor and process for the production of the intermediates

AN 2001:265443 CAPLUS

DN 134:281142

TI Process for the production of aspartyldipeptide ester derivatives, novel intermediates therefor and process for the production of the intermediates

IN Nagashima, Kazutaka; Aoki, Yuuichi; Takemoto, Tadashi; Amino, Yusuke; Funakoshi, Nao; Ono, Eriko

PA Ajinomoto Co., Inc., Japan

SO PCT Int. Appl., 39 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

	PA'	TENT	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D	ATE	
PI	WO	2001	.0252	 60		A1	-	2001	0412	1	WO 2	000-	 JP66:	 26		21	0000	 926
		W :	ΑE,															
			CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES,	FΙ,	GB,	GD,	GE,	GH,	GM,	HR,
			ΗU,	ID,	ΙL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,
			LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	RO,	RU,

SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG JP 1999-287398 Α 19991007 JP 1999-371284 19991227 AU 2000073219 Α5 20010510 AU 2000-73219 20000926 JP 1999-287398 19991007 Α JP 1999-371284 Ά 19991227 WO 2000-JP6626 20000926 EP 1231215 **A**1 20020814 EP 2000-961237 20000926 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL JP 1999-287398 Ά 19991007 JP 1999-371284 19991227 WO 2000-JP6626 20000926 US 2002133037 20020919 Α1 US 2002-117196 20020408 US 6794531 B2 20040921 JP 1999-287398 A 19991007 JP 1999-371284 A · 19991227 WO 2000-JP6626 A1 20000926 US 2004176472 **A**1 20040909 US 2004-796093 20040310 JP 1999-287398 19991007 JP 1999-371284 19991227 Α WO 2000-JP6626 A1 20000926 US 2002-177196 Al 20020621

OS CASREACT 134:281142; MARPAT 134:281142

GI

$$R^{2}$$
 R^{3}
 R^{4}
 R^{5}
 $CO_{2}H$
 O
 Ph
 I

$$R^2$$
 R^1 R^2 R^1 R^3 R^2 R^1 R^3 R^4 R^5 R^5 R^4 R^5 R^4 R^5 R^6 R^7

Industrial and efficient processes for producing aspartyldipeptide ester derivs. of general formula (I; R1-R5 = H, OH, C1-3 alkoxy, C1-3 alkyl, benzyloxy, C2-3 hydroxyalkyloxy; or R1 and R2 or R2 and R3 together represents methylenedioxy), which are expected to serve as sweetener (no data), comprise reductive alkylation of aspartame with propional dehydes or cinnamaldehydes of general formulas (II) and (III) in the presence of a catalyst. Particularly, described are an industrial and efficient process for producing N-[N-[3-(3-hydroxy-4-methoxyphenyl)propyl]~L-aspartyl]-Lphenylalanine 1-Me ester (IV) which is excellent as high sweetener; useful and advantageous intermediates for the process; and efficient processes for producing the intermediates. Thus, 5.89 g aspartame and 3.42 g

3-(3-hydroxy-4-methoxyphenyl)propional dehyde (preparation given) were added to 200 mL 80% aqueous methanol, stirred at 40° for a while, and hydrogenated in the presence of 1.78 10% Pd-C at 0.1 M Pa and 40° for 40 h to give 78.9% IV.

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 14.69 70.60 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL **ENTRY** SESSION CA SUBSCRIBER PRICE -2.10-2.10

FILE 'REGISTRY' ENTERED AT 12:36:14 ON 05 OCT 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ${\tt ZIC/VINITI}$ data file provided by ${\tt InfoChem.}$

STRUCTURE FILE UPDATES: 4 OCT 2004 HIGHEST RN 756793-93-8 DICTIONARY FILE UPDATES: 4 OCT 2004 HIGHEST RN 756793-93-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Examination Auxillary files\10796093\10796093 clmd cmpd isomer.str

chain nodes :
7 8 9 10 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
2-11 3-12 5-7 7-8 8-9 9-10 11-13 12-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-11 3-12 9-10 12-14
exact bonds :

5-7 7-8 8-9 11-13 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS

L4STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4

STR

Structure attributes must be viewed using STN Express query preparation.

=> search 14 exact full FULL SEARCH INITIATED 12:36:53 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 132 TO ITERATE

100.0% PROCESSED 132 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

1 SEA EXA FUL L4

=> d scan

1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Benzenepropanal, 4-hydroxy-3-methoxy- (9CI)

MF C10 H12 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> d 15

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 80638-48-8 REGISTRY

CN Benzenepropanal, 4-hydroxy-3-methoxy- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-(4'-Hydroxy-3'-methoxyphenyl)-1-propanal

CN 4-Propanal-2-methoxyphenol

FS 3D CONCORD

MF C10 H12 O3

LC STN Files: CA, CAPLUS, CASREACT, CHEMLIST, TOXCENTER, USPATFULL Other Sources: DSL**, EINECS**

(**Enter CHEMLIST File for up-to-date regulatory information)

DT.CA CAplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); RACT (Reactant or reagent)

RL.NP Roles from non-patents: BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

15 REFERENCES IN FILE CA (1907 TO DATE)

15 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 54.86 125.46 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -2.10

FILE 'CAPLUS' ENTERED AT 12:37:10 ON 05 OCT 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 5 Oct 2004 VOL 141 ISS 15 FILE LAST UPDATED: 4 Oct 2004 (20041004/ED) This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> 15
L6
           15 L5
=> 15/prep
           15 L5
       3205030 PREP/RL
            2 L5/PREP
1.7
                (L5 (L) PREP/RL)
=> d 17 m1-2 ti fbib abs
'M1-2' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'
The following are valid formats:
ABS ---- GI and AB
ALL ---- BIB, AB, IND, RE
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data and PI table (default)
CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
DALL ----- ALL, delimited (end of each field identified)
DMAX ----- MAX, delimited for post-processing
FAM ----- AN, PI and PRAI in table, plus Patent Family data
FBIB ----- AN, BIB, plus Patent FAM
IND ----- Indexing data
IPC ----- International Patent Classifications
MAX ----- ALL, plus Patent FAM, RE
PATS ---- PI, SO
SAM ----- CC, SX, TI, ST, IT
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
             SCAN must be entered on the same line as the DISPLAY,
             e.g., D SCAN or DISPLAY SCAN)
STD ----- BIB, IPC, and NCL
IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IMAX ----- MAX, indented with text labels
ISTD ----- STD, indented with text labels
OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ---- OBIB, indented with text labels
SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations
HIT ----- Fields containing hit terms
HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
             containing hit terms
HITRN ----- HIT RN and its text modification
HITSTR ----- HIT RN, its text modification, its CA index name, and
             its structure diagram
HITSEQ ----- HIT RN, its text modification, its CA index name, its
             structure diagram, plus NTE and SEQ fields
FHITSTR ---- First HIT RN, its text modification, its CA index name, and
            its structure diagram
FHITSEQ ---- First HIT RN, its text modification, its CA index name, its
             structure diagram, plus NTE and SEQ fields
```

KWIC ----- Hit term plus 20 words on either side OCC ----- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI, AU; BIB, ST; TI, IND; TI, SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number. ENTER DISPLAY FORMAT (BIB):end

=> d 17 1-2 ti fbib abs

- ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN L7
- Chemical composition of alkaline pulping products of lignin model ΤI compounds
- ΑN 1996:571131 CAPLUS
- 125:224831 DN
- Chemical composition of alkaline pulping products of lignin model TIcompounds
- Karpunin, I. I.; Muzychenko, M. P. ΑU
- Beloruss. Gos. Tech. Univ., Belarus CS
- Vestsi Akademii Navuk Belarusi, Seryya Khimichnykh Navuk (1996), (1), SO CODEN: VAKNEK; ISSN: 0002-3590
- PB Navuka i Tekhnika
- DTJournal
- LΑ Russian
- Alkaline pulping of lignin model compds. (guaiacylglycerol β -coniferyl AR ether, dehydrodiconiferyl alc., and pinoresinol) was carried out and several mono-, di-, tri-, tetra-, and pentameric products were separated and identified using paper chromatog., NMR and mass spectrometry.
- ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN L7
- Thermolytic decomposition of coniferyl alcohol TI
- 1992:553001 CAPLUS ΑN
- 117:153001 DN
- Thermolytic decomposition of coniferyl alcohol TI
- Masuku, Christopher P. ΑU
- Dep. Chem. Eng., Helsinki Univ. Technol., Espoo, SF-02150, Finland CS
- Journal of Analytical and Applied Pyrolysis (1992), 23(2), 195-208 SO CODEN: JAAPDD; ISSN: 0165-2370
- DTJournal
- LΑ English
- Thermal decomposition of coniferyl alc. was studied at 200-275° under an AB inert atmospheric to shed more light on the initial thermal reactions in the thermochem. conversion of lignin. In this temperature range, dimerization and oligomerization reactions dominated, whereas side chain C-C bond scission, dehydration, rearrangement, and H transfer reactions were partly obscured. The thermolytic reactions of the allylic side chain occurred more easily than those of the aryl-alkyl ether linkage. The primary aliphatic OH group was a site of transferable H. The major monoarom. products formed were dihydroconiferyl alc., coniferaldehyde, cis- and trans-isoeugenol, eugenol, and dihydroconiferaldehyde.

=> d 16 1-15 ti

- TI Fresh organically grown ginger (Zingiber officinale): composition and effects on LPS-induced PGE2 production
- L6 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Synthesis of N,N',N''-trisubstituted thiourea derivatives and their antagonist effect on the vanilloid receptor
- L6 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Carbon isotope ratio analysis of organic moieties from fossil mummified wood: establishing optimum conditions for off-line pyrolysis extraction using gas chromatography/mass spectrometry
- L6 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI The Relative Toxicity of Substituted Phenols Reported in Cigarette Mainstream Smoke
- L6 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Effect of pyrofoil composition on pyrolysis of lignin
- L6 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Process for producing and purifying aspartame derivative as sweetener
- L6 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Retention of lignin in seagrasses: angiosperms that returned to the sea
- L6 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Chemical composition of alkaline pulping products of lignin model compounds
- L6 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Thermolytic decomposition of coniferyl alcohol
- L6 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Ultrafiltration and pyrolysis gas chromatography mass spectrometry of chlorolignins in pulp mill effluent
- L6 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Evaluation of a tobacco fractionation procedure using pyrolysis mass spectrometry combined with multivariate analysis
- L6 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Characterization of tobacco lignin preparations by Curie-point pyrolysis-mass spectrometry and Curie-point pyrolysis-high-resolution gas chromatography/mass spectrometry
- L6 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Determination of phenols in coffee
- L6 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Topical cosmetics containing 1,7-diphenyl-4-hepten-3-one for skin disorder treatment
- L6 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparative recovery and analysis of the phenolic fractions from curing smoke. III. Separation and identification of mono- and dihydroxy compounds
- => d 16 14,15 ti fbib abs
- L6 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Topical cosmetics containing 1,7-diphenyl-4-hepten-3-one for skin disorder treatment

AN 1987:561391 CAPLUS

DN 107:161391

TI Topical cosmetics containing 1,7-diphenyl-4-hepten-3-one for skin disorder treatment

IN Miyahara, Reiji; Komazaki, Hisayuki; Magara, Tsunao; Sato, Etsuhisa; Hirao, Tetsuji

PA Shiseido Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
				**	
ΡI	JP 62099325	A2	19870508	JP 1985-239069	19851025
GI				JP 1985-239069	19851025

 \mathbb{R}^1

AB Topical cosmetics contain at least one compound selected from 1,7-diphenyl-4-hepten-3-one (I; R and R1 = H, OH, or OMe). A skin lotion consisted of 1,7-diphenyl-4-hepten-3-one 0.15, glycerin 4.0, 1,3-butylene glycol 4.0, EtOH 7.0, polyoxyethylene oleyl alc. 0.5, methylparaben 0.05, citric acid 0.01, Na citrate 0.1, a perfume 0.05, and H2O to 100% by weight

L6 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN

TI Preparative recovery and analysis of the phenolic fractions from curing smoke. III. Separation and identification of mono- and dihydroxy compounds

AN 1982:67395 CAPLUS

DN 96:67395

TI Preparative recovery and analysis of the phenolic fractions from curing smoke. III. Separation and identification of mono- and dihydroxy compounds

AU Wittkowski, Reiner; Toth, Lazlo; Baltes, Werner

CS Inst. Lebensmittelchem., Tech. Univ. Berlin, Berlin, D-1000, Fed. Rep. Ger.

SO Zeitschrift fuer Lebensmittel-Untersuchung und -Forschung (1981), 173(6), 445-57

CODEN: ZLUFAR; ISSN: 0044-3026

DT Journal

LA German

 ${\tt AB}$ To determine as completely as possible the composition of a phenolic extract obtained

by a mild procedure a monohydroxy- and dihydroxy-fraction were separated by treatment with a Na2BO3 solution By gas chromatog.-mass spectrometry-anal. of their trimethylsilyl-derivs. numerous new phenols were identified. The phenol extract of smoke contained about 20% of dihydroxybenzenes, the main constituents of which were represented by pyrocatechol and its 4- and 5-methyl-, 3- and 4-ethyl-, and 3-methoxy-derivs. The presence of 5 further dihydroxybenzenes was shown. By the technique described 119

=> d 16 6 ti fbib abs

- L6 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Process for producing and purifying aspartame derivative as sweetener
- AN 2001:185780 CAPLUS
- DN 134:223039
- TI Process for producing and purifying aspartame derivative as sweetener
- IN Amino, Yusuke; Yuzawa, Kazuko; Takemoto, Tadashi
- PA Ajinomoto Co., Inc., Japan
- SO PCT Int. Appl., 39 pp. CODEN: PIXXD2
- DT Patent
- Di Patent
- LA Japanese

ша	ou	Jui.	٠.
FAN.	CNT	1	

	PATENT NO.					KIND DATE			APPLICATION NO.					DATE				
ΡI	WO	2001	0180	 34		 A1		2001	0315	WO 2000-JP5665						 20000	 823	
		W:	ΑE,	AG,	AL,	AM,											, СН,	CN.
																	, GM,	
																	, LS,	
			LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT	, RO,	RU.
																	, UZ,	
								BY,							•			•
		RW:	GH,	GM,	KE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE	, CH,	CY,
			DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	ΙT,	LU,	MC,	NL,	PT,	SE	, BF,	ВJ,
			CF,	CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG			
											JP 1	999-	2534	98		A .	19990	907
	AU	2000	0672	73		A 5		2001	0410	1	AU 2	000-	6727:	3			20000	823
		*								1	JP 1	999-:	25349	98	1	A .	19990	907
										I	WO 2	000-	JP560	55	1	W :	20000	823
	US	2002	1473	61		A1		2002	1010	Ī	US 2	002-	91500)			20020	307
												999-					19990	
												000-				A1 :	20000	823
	US	2004	0490			A1		2004	0311			003-				:	20030	908
			* ***	•								999-:			i	Α	19990	907
							-					000-					20000	
										1	US 2	002-	91500)	1	A1	20020	307

OS CASREACT 134:223039

AB This document discloses the following: a method for industrially producing N-[N-[3-(3-methoxy-4-hydroxyphenyl)propyl]-L-α-aspartyl]-L-phenylalanine 1-Me ester which is useful as a sweetener, in particular, a process for producing the target compound in a high yield by the reductive alkylation reaction of aspartame with 3-(3-methoxy-4-hydroxyphenyl)propional dehyde or its derivative; a method of effectively purifying the target compound contaminated with impurities invading thereinto at various production stages (involving methods other than the above-described reductive alkylation), more particularly, a method of separating the target compound in the form of highly pure crystals; the crystals;

sweeteners containing the same; and utilization thereof in various products which are to be sweetened.

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> logoff hold
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
31.10
156.56

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

CA SUBSCRIBER PRICE

ENTRY -3.50

SESSION -5.60

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 12:53:12 ON 05 OCT 2004

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * SESSION RESUMED IN FILE 'CAPLUS' AT 13:18:52 ON 05 OCT 2004 FILE 'CAPLUS' ENTERED AT 13:18:52 ON 05 OCT 2004 COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	31.10	156.56
·		
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	\mathtt{TOTAL}
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-3.50	-5.60
=> file req		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
COST IN U.S. DOLLERS	ENTRY	SESSION
FULL ESTIMATED COST		
FULL ESTIMATED COST	31.54	157.00
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
, <u>2</u> ,	ENTRY	SESSION
CA SUBSCRIBER PRICE	-3.50	-5.60

FILE 'REGISTRY' ENTERED AT 13:19:24 ON 05 OCT 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 OCT 2004 HIGHEST RN 756793-93-8 DICTIONARY FILE UPDATES: 4 OCT 2004 HIGHEST RN 756793-93-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Examination Auxillary files\10796093\10796093 clmd cmpd homologs.str

chain nodes :

7 8 9 10 11 12 13 14

ring nodes :

1 2 3 4 5 6

chain bonds :

2-11 3-12 5-7 7-8 8-9 9-10 11-13 12-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

2-11 3-12 9-10 11-13

exact bonds :

5-7 7-8 8-9 12-14

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS

L8 STRUCTURE UPLOADED

=> d 18

L8 HAS NO ANSWERS

L8 STR

Structure attributes must be viewed using STN Express query preparation.

=> search 18 sss exact full
'SSS' IS NOT VALID HERE
For additional help, enter "HELP SEARCH".

=> search 18 sss full FULL SEARCH INITIATED 13:20:06 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 122173 TO ITERATE 100.0% PROCESSED 122173 ITERATIONS SEARCH TIME: 00.00.01

973 ANSWERS

L9 9'

973 SEA SSS FUL L8

=> d scan

L9 973 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C19 H22 O8 S

CI COM

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>

Uploading C:\Examination Auxillary files\10796093\10796093 clmd cmpd homologs $\tt Hfixed.str$

chain nodes :

7 8 9 10 11 12 13 14

ring nodes :

1 2 3 4 5 6

chain bonds :

2-11 3-12 5-7 7-8 8-9 9-10 11-13 12-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

2-11 3-12 9-10 11-13

exact bonds :

5-7 7-8 8-9 12-14

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Hydrogen count :

1:>= $\min 1$ 4:>= $\min 1$ 6:>= $\min 1$ 7:>= $\min 2$ 8:>= $\min 2$

9:>= minimum 1 13:>= minimum 3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS

=> d 110 L10 HAS NO ANSWERS L10 ST

Structure attributes must be viewed using STN Express query preparation.

0 ANSWERS

2 ANSWERS

=> search 110 sss sam
SAMPLE SEARCH INITIATED 13:22:35 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 6196 TO ITERATE

16.1% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 119202 TO 128638

PROJECTED ANSWERS: 0 TO

L11 0 SEA SSS SAM L10

=> search 110 sss full FULL SEARCH INITIATED 13:22:44 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 122173 TO ITERATE

100.0% PROCESSED 122173 ITERATIONS SEARCH TIME: 00.00.01

SEARCH TIME: 00.00.01

L12 2 SEA SSS FUL L10

=> d scan

L12 2 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN IN Benzeneacetaldehyde, 3-hydroxy-4-methoxy- (9CI)

MF C9 H10 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L12 2 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN IN Benzenepropanal, 3-hydroxy-4-methoxy- (9CI) MF C10 H12 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 313.36 470.36 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -5.60

FILE 'CAPLUS' ENTERED AT 13:23:54 ON 05 OCT 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 5 Oct 2004 VOL 141 ISS 15 FILE LAST UPDATED: 4 Oct 2004 (20041004/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 112 L13 11 L12 => d his (FILE 'HOME' ENTERED AT 12:21:11 ON 05 OCT 2004) FILE 'REGISTRY' ENTERED AT 12:21:23 ON 05 OCT 2004 STRUCTURE UPLOADED L11 SEARCH L1 EXACT FULL L2FILE 'CAPLUS' ENTERED AT 12:26:39 ON 05 OCT 2004 L3 3 L2 FILE 'REGISTRY' ENTERED AT 12:36:14 ON 05 OCT 2004 STRUCTURE UPLOADED L41 SEARCH L4 EXACT FULL L5 FILE 'CAPLUS' ENTERED AT 12:37:10 ON 05 OCT 2004 15 L5 L6 2 L5/PREP L7 FILE 'REGISTRY' ENTERED AT 13:19:24 ON 05 OCT 2004 STRUCTURE UPLOADED $\Gamma8$ 973 SEARCH L8 SSS FULL L9 STRUCTURE UPLOADED L10 0 SEARCH L10 SSS SAM L11L12 2 SEARCH L10 SSS FULL FILE 'CAPLUS' ENTERED AT 13:23:54 ON 05 OCT 2004 11 L12 L13 => 113 not 13 8 L13 NOT L3 T.14 => d 114 1-8 ti L14 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN Novel bicyclic and tricyclic pyrrolidine derivatives as GnRH antagonists L14 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN TINovel bicyclic and tricyclic pyrrolidine derivatives as GnRH antagonists ANSWER 3 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN The reaction of novocaine with the cobaltous halides L14 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN TIA new preparation of homoisovanillin L14 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN Mechanism of the Mohlan-Bischler indole synthesis. I. The mechanistic fate of carbonyl oxygen in the rearrangement of 2-anilino-1-phenyl-1-propanone L14 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN New preparation of homoisovanillin ANSWER 7 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN L145-Phenyl-2-penten-4-yn-1-ol and related compounds

L14 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN

Synthesis of 3-hydroxy-4-methoxyphenylacetaldehyde (homoisovanillin) and 3,4-dihydroxyphenylacetaldehyde (homoprotocatechualdehyde)

=> d 114 1-8 ti fbib abs:

L14 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN

Novel bicyclic and tricyclic pyrrolidine derivatives as GnRH antagonists ΤI

2002:409270 CAPLUS AN

137:6173 DN

ΤI Novel bicyclic and tricyclic pyrrolidine derivatives as GnRH antagonists

Peng, Ge; Gallop, Mark A.; Chernov-Rogan, Tania; Yanofsky, Stephen D.; Pelletier, Jeffrey Claude; Green, Daniel Michael

PA SO DT LA	USA U.S. Pat. Appl. CODEN: USXXCO Patent English	Publ., 48	pp., Cont	-in-part of U.S. Ser. N	No. 633,025.		
	CNT 3 PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI	US 2002065309	A1	20020530		20010518 P 19990804 A2 20000804		
	WO 2002011732 WO 2002011732	A1 C1	20020214 20020620	WO 2001-US24506	20010803		
	W: AE, AG, CO, CR, HR, HU, LT, LU, RU, SD, YU, ZA, RW: GH, GM, DE, DK,	AL, AM, AT CU, CZ, DE ID, IL, IN LV, MA, MD SE, SG, SI ZW, AM, AZ KE, LS, MW ES, FI, FR	AU, AZ, F C, DK, DM, I I, IS, JP, F D, MG, MK, N C, SK, SL, T G, BY, KG, F J, MZ, SD, S R, GB, GR, I	BA, BB, BG, BR, BY, BZ, DZ, EE, ES, FI, GB, GD, KE, KG, KP, KR, KZ, LC, MN, MW, MX, MZ, NO, NZ, IJ, TM, TR, TT, TZ, UA, KZ, MD, RU, TJ, TM SL, SZ, TZ, UG, ZW, AT, IE, IT, LU, MC, NL, PT, GQ, GW, ML, MR, NE, SN,	GE, GH, GM, LK, LR, LS, PL, PT, RO, UG, UZ, VN, BE, CH, CY, SE, TR, BF,		
ΡΔͲϝ	AU 2001081067	A 5	20020218	US 2000-633025 US 2001-860810 AU 2001-81067 US 2000-633025	A 20000804 A 20010518 20010803 A 20000804 A 20010518 W 20010803		
FAN	2001:582116 PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI	WO 2001057288 W: JP, SG, RW: AT, BE,	A1 UA	20010809	WO 2000-US21175	20000803		
	PT, SE EP 1198608 R: AT, BE, IE, FI,		20020424 K, ES, FR, (US 1999-147233P US 2000-621757 EP 2000-952447 GB, GR, IT, LI, LU, NL,	P 19990804 A 20000724 20000803 , SE, MC, PT,		
	JP 2003521584	Т2	20030715	US 1999-147233P US 2000-621757 WO 2000-US21175 JP 2001-555910 US 1999-147233P US 2000-621757 WO 2000-US21175	P 19990804 A 20000724 W 20000803		
EAN	2002-122704			2000 0000			

FAN 2002:122794

	PATENT NO.				KIND DATE			APPLICATION NO.						DATE			
ΡI	WO 2002 WO 2002				A1 C1		2002 2002			WO .	 2001-	 US24	506			20010	803
															~-	~	
	W:															., СН,	
		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE	, ES,	FΙ,	GB,	GD,	GE	, GH,	GM,
		HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG	, KP,	KR,	ΚZ,	LC,	LK	, LR,	LS,
		LT,	LU,	LV,	MA,	MD,	MG,	MK,	·MN,	MW	, MX,	MZ,	NO,	NZ,	PL	, PT,	RO,
																, UZ,	
			•					•	•		, RU,	•		•			-
	RW:	•	•	•	•	•	•	•	•		•			AT.	BE	, CH,	CY.
		•	•	•	•	•	•	•	•		, ,	•	•	•		, TR,	
		•							•		, ML,	•	•	•			,
		20,	~~ <i>,</i>	,	,	0.17	011,	01.,						•		20000	804
															_		
	110 2002	0653	00		7.1		20020530			US 2001-860810 US 2001-860810							
	US 2002	000,3	09		A 1		2002	0530								20010	
											1999-					19990	
																20000	
_	AU 2001	0810	67		A 5		2002	0218	i	AU :	2001-	8106	7			20010	803
									1	US :	2000-	6330	25		A	20000	804
									1	US :	2001-	8608	10		A	20010	518
									Ţ	WO :	2001-	US24	506	1	W	20010	803
os	MARPAT	137:	6173														
GΙ																	

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Title compds. I [L1, L2 and L3 are independently linking groups; m, n, q are independently 0 or 1; Y = (H)a and Z = (OH)b, c is an optional single bond, wherein, when c = single bond, a and b are both 0, when c is absent, a and b are both 1; Q = O or S; X = N or CH; R1 and R2 are either (un) substituted hydrocarbyl (the same or different), or R1 and R2 are linked to form a 5- or 6-membered ring optionally containing 1-3 heteroatoms (selected from N, O and S); R3 = cyclic structure of 1-3 rings that may be fused or linked, wherein 1 or more of the rings maybe aromatic and/or heterocyclic; R4, R5, R6, R7 and R8 are independently selected from H, halo, OH, alkyl, alkenyl, alkoxy, etc., and further, when two of R4, R5, R6, R7 and R8 are ortho to each other, they may together form a 5- or 6-membered cyclic structure containing 0-2 heteroatoms; R9 and R10 = H, halo, OH, alkyl, alkenyl, alkynyl, alkoxy, amino, lower alkyl-substituted amino, nitro, nitrile and carboxyl], their preparation, methods of use and pharmaceutical compns. as antagonists of the GnRH receptor are disclosed. Thus, II was prepared in seven steps in 25% overall yield from resin bound α -BOC- β -FMOC-diaminopropionic acid with the bicyclic pyrrolidine core being formed by a zinc catalyzed intramol. cyclization. Evaluation of I for binding inhibition of human GnRH receptors provided IC50 values ranging from 35-1500 nM.

- L14 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Novel bicyclic and tricyclic pyrrolidine derivatives as GnRH antagonists
- AN 2002:122794 CAPLUS
- DN 136:167362
- TI Novel bicyclic and tricyclic pyrrolidine derivatives as GnRH antagonists
- IN Peng, Ge; Gallop, Mark A.; Chernov-Rogan, Tania; Yanovsky, Stephen; Pelletier, Jeffrey Claude; Green, Daniel Michael
- PA Glaxo Group Limited, UK
- SO PCT Int. Appl., 118 pp. CODEN: PIXXD2
- DT Patent
- LA English

```
FAN.CNT 3
                                                 APPLICATION NO.
                           KIND
     PATENT NO.
                                     DATE
                                                                               DATE
                            ----
                                     _____
                                                   ______
      _____
                                                                              _____
                                                 WO 2001-US24506
                                                                               20010803
     WO 2002011732
                             A1
                                     20020214
PI
                              C1
     WO 2002011732
                                     20020620
          W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
               CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
          RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                                   US 2000-633025 A 20000804
                                                   US 2001-860810
                                                                           A 20010518
                                                   US 2001-860810
     US 2002065309
                              Α1
                                     20020530
                                                   20010518
P 19990804
US 2000-633025 A2 20000804
AU 2001-81067
                                                                               20010518
     AU 2001081067
                                     20020218
                              Α5
                                                   US 2000-633025
                                                                       A 20000804
A 20010518
                                                   US 2001-860810
                                                                       W 20010803
                                                   WO 2001-US24506
PATENT FAMILY INFORMATION:
     2001:582116
                                     DATE APPLICATION NO.
     PATENT NO.
                            KIND
                                                                              DATE
                            _----
     WO 2001057288
                             A1
                                     20010809
                                                WO 2000-US21175
                                                                               20000803
          W: JP, SG, UA
          RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
               PT. SE
                                                   US 1999-147233P
                                                                         P 19990804
                                                 US 2000-621757 A 20000724
EP 2000-952447 20000803
     EP 1198608
                              A1
                                     20020424
          R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
               IE, FI, CY
                                                   US 1999-147233P
                                                                         P 19990804
                                                                        A 20000724
                                                   US 2000-621757
                                                   WO 2000-US21175
                                                                           W 20000803
     JP 2003521584
                              T2
                                     20030715
                                                   JP 2001-555910
                                                                               20000803
                                                                         P 19990804
                                                   US 1999-147233P
                                                                       A 20000724
W 20000803
                                                   US 2000-621757
                                                   WO 2000-US21175
     2002:409270
FAN
     PATENT NO.
                             KIND
                                     DATE
                                                   APPLICATION NO.
                                                                               DATE
     -----
                             ____
                                     _____
                                                   ______
                                                   US 2001-860810
PT
     US 2002065309
                             A1
                                     20020530
                                                                               20010518
                                                   US 1999-147233P P 19990804
US 2000-633025 A2 20000804
     WO 2002011732
                                                   WO 2001-US24506
                             A1
                                     20020214
                                                                               20010803
     WO 2002011732
                             C1
                                     20020620
              AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
               CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM,
               HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO,
               RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN,
               YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
          RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
               DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
               BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                                   US 2000-633025 A 20000804
                                                   US 2001-860810
                                                                         A 20010518
     AU 2001081067
                            A5
                                                                              20010803
                                     20020218
                                                 AU 2001-81067
```

US 2000-633025 A 20000804 US 2001-860810 A 20010518 WO 2001-US24506 W 20010803

OS MARPAT 136:167362

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Title compds. I [L1, L2 and L3 are independently linking groups; m, n, qare independently 0 or 1; Y = (H)a and Z = (OH)b, c is an optional single bond, wherein, when c = single bond, a and b are both 0, when c is absent, a and b are both 1; Q = 0 or S; X = N or CH; R1 and R2 are either (un) substituted hydrocarbyl (the same or different), or R1 and R2 are linked to form a 5- or 6-membered ring optionally containing 1-3 heteroatoms (selected from N, O and S); R3 = cyclic structure of 1-3 rings that may be fused or linked, wherein 1 or more of the rings maybe aromatic and/or heterocyclic; R4, R5, R6, R7 and R8 are independently selected from H, halo, OH, alkyl, alkenyl, alkoxy, etc., and further, when two of R4, R5, R6, R7 and R8 are ortho to each other, they may together form a 5- or 6-membered cyclic structure containing 0-2 heteroatoms; R9 and R10 = H, halo, OH, alkyl, alkenyl, alkynyl, alkoxy, amino, lower alkyl-substituted amino, nitro, nitrile and carboxyl], their preparation, methods of use and pharmaceutical compns. as antagonists of the GnRH receptor are disclosed. Thus, II was prepared in seven steps in 25% overall yield from resin bound α -BOC- β -FMOC-diaminopropionic acid with the bicyclic pyrrolidine core being formed by a zinc catalyzed intramol. cyclization. Evaluation of I for binding inhibition of human GnRH receptors provided IC50 values ranging from 35-1500 nM.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN

TI The reaction of novocaine with the cobaltous halides

AN 1959:62416 CAPLUS

DN 53:62416

OREF 53:11289e-q

TI The reaction of novocaine with the cobaltous halides

AU Khakimov, Kh. Kh.; Azizov, M. A.

CS Pharm. Inst., Tashkent

SO Doklady Akademii Nauk UzSSR (1958), (No. 10), 31-4 CODEN: DANUAO; ISSN: 0134-4307

DT Journal

LA Unavailable

AB The halide salts of novocaine (C13H20O2N2) (I) form 2 series of salts with COX2. Compds. of the 1st series were prepared by dropwise addition of 1 part saturated aqueous COX2 to 3 parts saturated aqueous solution of I.HX. The precipitate was washed

with alc. then ether: CoCl2.2I.2HCl, bright blue, m. 184°, conductivity 425, solubility 50 g./100 g. H2O; CoBr2.2I.2HBr, greenish blue, m. 149°, conductivity 398, solubility 45 g./100 g. H2O. Compds. of the 2nd series were prepared

by mixing equivalent amts. of CoX2 and I, both dissolved in concentrated solns. of

the corresponding acid. CoCl2.I.2HCl, bright blue, m. 223°, conductivity 771, solubility 47 g./100 g. H2O; CoBr2.I.2HBr, greenish blue, m. 212°, conductivity 611, solubility 190 g./100 g. H2O; CoI2.I.2HI.2H2O, green, m. 125, conductivity

743, solubility 300 g./100 g. H2O. In aqueous and alc. solution the free base did not

form complex salts.

- L14 ANSWER 4 OF 8, CAPLUS COPYRIGHT 2004 ACS on STN A new preparation of homoisovanillin AN 1959:62415 CAPLUS DN 53:62415 OREF 53:11289e A new preparation of homoisovanillin Hermanek, S.; Stanek, J. ΑU Collection of Czechoslovak Chemical Communications (1959), 24, 1366-8 SO CODEN: CCCCAK; ISSN: 0010-0765 DTJournal Unavailable LA AB See C.A. 52, 10941c. ANSWER 5 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN T.14 Mechanism of the Mohlan-Bischler indole synthesis. I. The mechanistic fate TΤ of carbonyl oxygen in the rearrangement of 2-anilino-1-phenyl-1-propanone ΑN 1959:62414 CAPLUS 53:62414 DN OREF 53:11289b-e Mechanism of the Mohlan-Bischler indole synthesis. I. The mechanistic fate of carbonyl oxygen in the rearrangement of 2-anilino-1-phenyl-1-propanone Nelson, K. LeRoi; Seefeld, Ralph L. ΑIJ CS Wayne State Univ., Detroit, MI Journal of the American Chemical Society (1958), 80, 5957-9 SO CODEN: JACSAT; ISSN: 0002-7863 DTJournal Unavailable LA OS CASREACT 53:62414 The mechanism of rearrangement of PhNHCHMeBz (I) to AcCHPhNHPh (II) in the AR presence of PhNH3Br (III) or pyridine-HBr (IV) was investigated with use of O18 as tracer. I (0.01 mole) and 0.01 mole III in 25 ml. 95% EtOH (made up with H2O containing 1.4 atom-% O18) refluxed 8.5 hrs. under N gave 0.55 g. I and 1.09 g. II containing 0.68 and 0.36 atom-\$ excess 018, resp. I and IV refluxed similarly 20 hrs. gave 1.13 g. I and 0.38 g. III containing 0.84 and 0.16 atom-% excess 018. II and III refluxed 4 hrs. gave 0.14 g. I, whereas II and IV gave no I after 12 hrs. I refluxed with p-ClC6H4NH3Br, m. 243-5°, showed amine exchange and gave p-ClC6H4NHCHPhAc, m. 129-31°. The results showed that there is exchange of O between carbonyl and solvent, exclusive of any rearrangement, and that there is no important O exchange directly associated with rearrangement of I to II or II to I. The reaction must involve intramol. migration of the carbonyl O and cannot proceed by the mechanism proposed by Cowper and Stevens (C.A. 42, 147c). A new mechanism is proposed involving addition of catalyst to the carbonyl C and formation of an intermediate epoxy structure. L14 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN New preparation of homoisovanillin TI1958:61002 CAPLUS AN 52:61002 DN OREF 52:10941c-e New preparation of homoisovanillin TIΑU Hermanek, Stanislav; Stanek, Jan CS Tech. Univ., Prague Chemicke Listy pro Vedu a Prumysl (1958), 52, 355-6 SO CODEN: CLPRAN; ISSN: 0366-6832 DTJournal
- In Unarrail
- LA Unavailable
- OS CASREACT 52:61002
- AB Ozonization of the benzyl ether of chavibetol (I), subsequent hydrogenation of the ozonide, and hydrogenolysis of the resulting benzyl ether (II) of homoisovanillin (III) gave III in 49% over-all yield.

Similarly was prepared homoveratric aldehyde (IV). Passing 6 hrs. a stream of dry O containing 3% O3 at 100 ml./min. through 15 g. I in 200 ml. AcOEt cooled with dry CO2 in Me2CO, adding 3 g. 5% Pd/Al2O3, hydrogenating 3 hrs., and evaporating the solvent gave crude II. This dissolved in 450 ml. MeOH and hydrogenated over 3 g. catalyst gave after 4 hrs. 5.1 g. III, b0.2 117-22°; semicarbazone, m. 182°. Similar treatment of 10 g. eugenol Me ether gave 5.1 g. IV, b0.3 118-23°; semicarbazone, m. 162-3°. IV (7.2 g.) kept 2 days with 32 g. 2% HCl-absolute MeOH, the mixture boiled 15 min., diluted with 5 vols. H2O, extracted with Et2O, the extract shaken 15 min. with 2 g. NH2OH.HCl and 1.6 g. KOH in 15 ml. ice water, the solvent evaporated, and the oil distilled gave 4.5 g. di-Me acetal IV, b0.3 112-16°. Attempts at demethylation of the di-Me acetal (4.5 g.) by treatment with Na in liquid NH3 failed, yielding 3.5 g. recovered starting compound and 0.9 g. mixture containing guaiacol. ANSWER 7 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN L145-Phenyl-2-penten-4-yn-1-ol and related compounds 1958:61001 CAPLUS 52:61001 OREF 52:10940h-i,10941a-c 5-Phenyl-2-penten-4-yn-1-ol and related compounds Jacobs, Thomas L.; Dankner, David; Dankner, Arlyn R. Univ. of California, Los Angeles Journal of the American Chemical Society (1958), 80, 864-6 CODEN: JACSAT; ISSN: 0002-7863 Journal Unavailable CASREACT 52:61001 Epichlorohydrin (102 g.) added dropwise during about 0.5 h. to 2 mol PhC.tplbond.CNa in 2.3 l. liquid NH3, refluxed 7 h. with stirring, treated with 118 g. NH4Cl in 3 portions and then with 1 l. Et2O, the NH3 evaporated overnight with stirring, the residual Et20 solution filtered, the residue washed with Et20 and dissolved in H2O, the aqueous solution extracted with Et20, and the combined Et2O solns. worked up gave about 0.8 mol PhC.tplbond.CH, 55.2 g. α -benzylfuran, b0.001 50-2°, n25D 1.5411, and 58.6 g. PhC.tplbond.CCH:CHCH2OH (I), b0.001 92-7°, n25D 1.6158. CrO3 (15.8 g.) and 25.3 g. concentrated H2SO4 diluted with H2O to 79 cc., the solution added dropwise with stirring to 17.9 g. I in 70 cc. Me2CO during 1 h. at about 15%, the mixture stirred 1 h. at 15°, poured onto crushed ice, and extracted with Et20, and the extract extracted with aqueous NaHCO3, dried, and worked up gave 9.7 g. PhC.tplbond.CCH:CHCHO(II), b0.001 62°, n25D 1.6422; the aqueous NaHCO3 extract gave 0.4 g. PhC:CCO2H, m. 130-3°. II (12.1 g.) in EtOH added to Ag20 (from 72.7 g. AgNO3 and 12.4 g. NaOH) in 400 cc. H2O and shaken 22 h., the Ag salt treated with aqueous NaOH, and the resulting Na salt treated with dilute H2SO4 yielded PhC.tplbond.CCH:CHCO2H (III), m. $147\text{--}8.6\,^{\circ}$ (pentane). III (0.3 g.) in 4.46 g. glacial AcOH and 4.46 g. concentrated H2SO4 warmed 5 h. on the steam bath, kept at room temperature overnight, diluted with H2O, and cooled, and the solid product dissolved in Et20, washed with H20, dried, and evaporated gave 0.28 g. phenylcoumalin (IV), m. 66-7° (pentane). PhC.tplbond.CCH:C(CO2H)2, m. 200-18°, refluxed 18 h. in p-xylene yielded the 3-CO2H derivative of IV, m. 218°. L14ANSWER 8 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN Synthesis of 3-hydroxy-4-methoxyphenylacetaldehyde (homoisovanillin) and 3,4-dihydroxyphenylacetaldehyde (homoprotocatechualdehyde) 1941:568 CAPLUS 35:568 OREF 35:94e-i,95a-h

of

TI

ΑN

DN

TΤ

ΑIJ

CS

SO

DT

LΑ OS

AB

AN

DN

```
Synthesis of 3-hydroxy-4-methoxyphenylacetaldehyde (homoisovanillin) and
     3,4-dihydroxyphenylacetaldehyde (homoprotocatechualdehyde)
ΑU
     Schopf, Clemens; Brass, Eva; Jacobi, Ernst; Jorde, Walter; Mocnik, Walter;
     Neuroth, Ludwig; Salzer, Walter
SO
     Ann. (1940), 544, 30-62
DT
     Journal
LΑ
     Unavailable
     The following aldehydes have been synthesized because of their importance
AΒ
     as building units in the biogenesis of plant substances, especially the
     alkaloids, and for a study of their condensation with such compds. as
     3,4-(HO)2C6H3CH2CH2NH2 under physiol. conditions. Details are given of
     the preparation of chavibetol, 3,4-HO(MeO)C6H3CH2CH:CH2 (I), from eugenol (II)
     Me ether by the use of MeMgI in xylene at 160-80° (2 h.); unchanged
     II can be removed in part by cooling a solution of 42 g. of the mixture in 120
     cc. absolute EtOH containing 19 g. KOH, whereby the K salt of II seps.; the
alc.
     filtrate gives 15.5 g. of crude I which can be further purified through
     the Bz derivative, m. 49.5°. The crude I may be treated with PhCH2Cl
     and K2CO3 in MeOH (boiling 20 h.) and the benzyl ether (III) of I, m.
     48°, crystallized from MeOH; the yield of pure III from pure I is 82%;
     30 g. crude I yields 33 g. pure III. III (5.1 g.) in 60 cc. C6H6, heated
     20 h. with a mixture of 10.1 g. BzOAg and 5.7 g. I in 35 cc. C6H6
     (previously shaken for 15 min. and then warmed on the water bath for 5
     min.), the AgI filtered off, the C6H6 removed by evaporation, the residue
     dissolved in 100 cc. MeOH, saponified with 3.2 g. Na in 32 cc. MeOH, the
     mixture extracted with CHCl3 and crystallized from AcOEt, gives 4.2 g. of
     benzylchavibetol glycol (IV), b0.04 215-20°, m. 110°. IV
     was also prepared by the following method. 3,4-PhCH2O(MeO)C6H3CH2CO2H with
     SOC12 (must be purified over beeswax to give a crystalline product) (boiling in
     C6H6 for 8 h.) or with PC15 (in C6H6, 0.5 h. at 0^{\circ}) gives the acid
     chloride which, without purification, reacts with CH2N2 in ether to give 81% of
     the diazo ketone, C17H16O3N2, yellow, m. 86°; addition of 10 g. to 20
     cc. AcOH at 60-70° yields 77% of the acetoxy ketone, C19H2OO5, m.
     106°, which is reduced by (iso-PrO)3Al in iso-PrOH to IV (94%
     yield). Shaking IV in MeOH with PdCl2-BaSO4 in a H atmospheric gives
chavibetol
     glycol, m. 86°. Details are given of the preparation of
     3,4-PhCH2O(MeO)C6H3CH2COCO2H (V) (cf. Robinson and Sugasawa, C. A. 26,
     1289); Me ester, m. 148-50°. Catalytic reduction of V yields
     \alpha-hydroxy-\beta-(3-hydroxy-4-methoxyphenyl)propionic acid, (VI), m.
     170^{\circ} (Me ester, m. 62^{\circ}); Pb(OAc)4 splits off 55\% of the
     calculated amount of CO2 but the aldehyde could not be isolated.
     of V in 50% hot AcOH with Zn (boiling 1 h.) gives 5.2 g. of the 3-benzyl
     ether of VI, m. 129-30°; CH2N2 gives the Me ester (VII), m.
     87°. VII (6.3 g.) and MeMgI give 5.9 g. of the glycol (VIII),
     3,4-PhCH2O(MeO)C6H3CH2CH(OH)CMe2OH, m. 86°. VIII with Pb(OAc)4 in
     C6H6 gives a nearly quant. yield of 3-benzyloxy-4-
    methoxyphenylacetaldehyde (IX), b0.01 155° (bath temperature);
     semicarbazone, m. 143-4°; 2,4-dinitrophenylhydrazone, m.
     151-2°. IV with Pb(OAc)4 in hot C6H6 gives 90% of IX. With Pd in
    MeOH IX gives 3-hydroxy-4-methoxyphenylacetaldehyde (X), b0.05
    110-15° (bath temperature); 0.53 g. is soluble in 50 cc. H2O; semicarbazone,
    m. 182-3^{\circ}. X is stable for 24 h. at room temperature in an acetate
    buffer solution at pH 3 and 4; only slight decomposition occurs at pH 5 and 6
but
     considerable decomposition occurs at pH 7; at pH 8 X is completely decomposed
in
     24 h. This stability compares with that of 3,4-CH2O2C6H3CH2CHO.
     3,4-(HO)2C6H3CH2CH:CH2 (XI) (prepared in a poor yield from o-C6H4(OH)2 and
     in 33% yield from eugenol Me ether with MeMgI) (28 g.) in 140 cc. Me2CO
     and 130 g. K2CO3, treated dropwise with 87 cc. PhCH2Cl and heated 20-2 h.
     on the water bath, gives, after purification of the C6H6 solution by
adsorption on
```

Al203, 75% of 3,5-dibenzyloxyallylbenzene (XI), m. 37-8°. Treatment of 6.6 g. XI with BzOAg and I in C6H6 as above, gives 75% of 1,2-dihydroxy-3-(3',4'-dibenzyloxyphenyl)propane, m. 82-3° Pb(OAc)4 in hot AcOH gives after 20 min. of reaction time 3,4-dibenzyloxyphenylacetaldehyde, an oil, whose semicarbazone m. 158°; catalytic reduction with an active Pd in MeOH gives 3,4-dihydroxyphenylacetaldehyde (XII), which could not be distilled; semicarbazone, m. 200-1°; 2,4-dinitrophenylhydrazone, m. 169-70°. XII is stable for 12 h. at 25° at pH 3 and 4 but rapidly decomps. at pH 7 and 8, giving a red solution, probably the o-quinone. 3,4-Methylenedioxyphenylpyruvic acid (XIII) gives a Me ester, m. 130-1°. Catalytic reduction of XIII with PtO2 in dilute aqueous Na2CO3 gives α -hydroxy- β -(3,4-methylenedioxyphenyl)propionic acid (XIV), m. 101°; Pb(OAc)4 in C6H6 or AcOH gives 34 or 31% of homopiperonal (XV). The Me ester of XIV, m. 39°, with MeMgI yields 2-methyl-2,3-dihydroxy-4-(3',4'-methylenedioxyphenyl)butane, m. 106°; with Pb (OAc)4 this gives Me2CO and a good yield of XV. 2,3-Ac2C6H3CH2CH:CH2 (m. 65°) (1 g.) with N BzO2H in CHCl3 (5 days) gives 2 g. of the oxide [1,2-oxido-3-(2',3'-diacetoxyphenyl)propane], b0.05 160° (bath temperature), m. 86°; the corresponding oxide of 3,4-Ac2C6H3CH2CH:CH2 could not be distilled or crystallized Acetyleugenol

g.) gives 12.5 g. of the oxide [1,2-oxido-3-(3'-methoxy-4'-acetoxyphenyl)propane], b0.05 133°, m. 50-2°; refluxing with 10% AcOH gives acetyleugenol glycol, b0.03 168°. The dibenzyl ether (m. 92-3°, 73% yield) with hippuric acid, Ac2O and AcONa, heated 2 h. on the water bath, gives 60% of 2-phenyl-4-(3',4'-dibenzyloxybenzylidene)oxazolone, yellow, m. 156-7°; it could not be hydrolyzed by 10% NaOH or KOH. Isoferulic acid (XVI) and Br in AcOH give 3-hydroxy-4-methoxy- ω -bromostyrene (XVII), m. 95-6°; the Ac derivative of XVI with Br in CHC13 gives the Ac derivative of XVII, m. 101-2°. 3,4-Dimethoxy- ω -bromostyrene, heated with EtONa for 2 h. at 180-5°, gives 3,4-dimethoxyphenylacetylene, b15 130°, m. 73-4. ω -(3,4-Diacetoxyphenyl)- β -acetoxyethanone, on reduction with Zn in AcOH at 70°, gives 3,4-Ac2C6H3Ac, m. 86°. The compds. of Voswinkel (C. A. 4, 769), 3,4-Ac2C6H3CH2CH2OH and 3,4-Ac2C6H3CH2CHO, do not exist.

=> 113/prep FIELD CODES CANNOT BE CHANGED HERE You may have tried to apply a field code to a term that already has a field code. You can only add a field code to a term that has no field code appended to it.

=> 112/prep

11 L12

3205030 PREP/RL

L15

4 L12/PREP

(L12 (L) PREP/RL)

=> d 115 1-4 ti ti

- L15 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Novel bicyclic and tricyclic pyrrolidine derivatives as GnRH antagonists
- TI Novel bicyclic and tricyclic pyrrolidine derivatives as GnRH antagonists
- L15 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Novel bicyclic and tricyclic pyrrolidine derivatives as GnRH antagonists
- TI Novel bicyclic and tricyclic pyrrolidine derivatives as GnRH antagonists
- L15 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Process for producing cinnamyl aldehyde derivatives and use thereof as

- intermediate for aspartame derivative
 Process for producing cinnamyl aldehyde derivatives and use thereof as
 intermediate for aspartame derivative
- L15 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Process for the production of aspartyldipeptide ester derivatives, novel intermediates therefor and process for the production of the intermediates
- TI Process for the production of aspartyldipeptide ester derivatives, novel intermediates therefor and process for the production of the intermediates

=> save temp 115 aspcmpds/a
ANSWER SET L15 HAS BEEN SAVED AS 'ASPCMPDS/A'

=>

---Logging off of STN---

Connection closed by remote host END

Unable to generate the STN prompt. Exiting the script...

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America

NEWS 2 "Ask CAS" for self-help around the clock

NEWS 3 Jul 12 BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS

NEWS 4 AUG 02 IFIPAT/IFIUDB/IFICDB reloaded with new search and display

NEWS 5 AUG 02 CAplus and CA patent records enhanced with European and Japan

Patent Office Classifications
NEWS 6 AUG 02 The Analysis Edition of STN Express with Discover!
(Version 7.01 for Windows) now available

NEWS 7 AUG 27 BIOCOMMERCE: Changes and enhancements to content coverage

NEWS 8 AUG 27 BIOTECHABS/BIOTECHDS: Two new display fields added for legal status data from INPADOC

NEWS 9 SEP 01 INPADOC: New family current-awareness alert (SDI) available

NEWS 10 SEP 01 New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!

NEWS 11 SEP 01 New display format, HITSTR, available in WPIDS/WPINDEX/WPIX

NEWS 12 SEP 14 STN Patent Forum to be held October 13, 2004, in Iselin, NJ

NEWS 13 SEP 27 STANDARDS will no longer be available on STN

NEWS 14 SEP 27 SWETSCAN will no longer be available on STN

NEWS EXPRESS JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT

MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004

NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items

NEWS PHONE Direct Dial and Telecommunication Network Access to STN

NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 08:22:00 ON 06 OCT 2004

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

0.21

0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 08:22:16 ON 06 OCT 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file

provided by InfoChem.

STRUCTURE FILE UPDATES: 4 OCT 2004 HIGHEST RN 756793-93-8

STRUCTURE FILE UPDATES: 4 OCT 2004 HIGHEST RN 756793-93-8 DICTIONARY FILE UPDATES: 4 OCT 2004 HIGHEST RN 756793-93-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>

Uploading C:\Examination Auxillary files\10796093\10796093 clmd cmpd protected H fixed.str

12 4 7 8 9 10 13 2 6

chain nodes :
7 8 9 10 11 12 13
ring nodes :

1 2 3 4 5 6

chain bonds :

2-11 3-12 5-7 7-8 8-9 9-10 11-13

ring bonds :

1-2 1-6 2-3 3-4 4-5

exact/norm bonds :

2-11 3-12 9-10 11-13

exact bonds :

5-7 7-8 8-9

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Hydrogen count:

1:>= minimum 1 4:>= minimum 1 6:>= minimum 1 7:>= minimum 2 8:>= minimum 2 9:>= minimum 1 13:>= minimum 3

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS

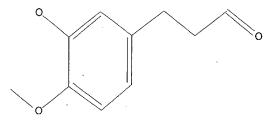
L1STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1

STR



Structure attributes must be viewed using STN Express query preparation.

=> search 11 sss sam

SAMPLE SEARCH INITIATED 08:22:44 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 4124 TO ITERATE

24.2% PROCESSED

1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

> BATCH **COMPLETE**

PROJECTED ITERATIONS:

78630 TO 86330

PROJECTED ANSWERS:

0 TO

L2 0 SEA SSS SAM L1

=> search l1 sss full

FULL SEARCH INITIATED 08:22:53 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 81536 TO ITERATE

100.0% PROCESSED 81536 ITERATIONS

SEARCH TIME: 00.00.02

8 ANSWERS

=> d scan

L3 8 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Benzenepropanal, 3-[2-(4-fluorophenyl)ethoxy]-4-methoxy- (9CI)

MF C18 H19 F O3

OMe
$$O-CH_2-CH_2$$
 OHC-CH₂-CH₂

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):8

L3 8 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Benzenepropanal, 4-methoxy-3-(phenylmethoxy)- (9CI)

MF C17 H18 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 8 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Benzenepropanal, 3-(cyclopentyloxy)-4-methoxy- (9CI)

MF C15 H20 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 8 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Benzenepropanal, 4-methoxy-3-[2-(4-methyl-5-thiazolyl)ethoxy]- (9CI)

MF C16 H19 N O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 8 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Benzenepropanal, 4-methoxy-3-[4-[(phenylthio)methyl]phenoxy]- (9CI)

MF C23 H22 03 S

$$\begin{array}{c} \text{OMe} \\ \\ \text{OHC-CH}_2\text{-CH}_2 \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 8 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Benzenepropanal, 3-(cyclopentylmethoxy)-4-methoxy- (9CI)

MF C16 H22 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 8 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Benzenepropanal, 3-hydroxy-4-methoxy- (9CI)

MF C10 H12 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 8 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Benzenepropanal, 3,4-dimethoxy- (9CI)

MF C11 H14 O3

MeO
$$_{\mathrm{CH_2-CH_2-CHO}}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 156.68 156.89

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 08:24:42 ON 06 OCT 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 6 Oct 2004 VOL 141 ISS 15 FILE LAST UPDATED: 4 Oct 2004 (20041004/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 13

L4

27 L3

=> d 17-27 ti

- L4 ANSWER 17 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI A practical iodination of aromatic compounds using tetrabutylammonium peroxydisulfate and iodine
- L4 ANSWER 18 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Utilization of the Intramolecular Cycloaddition-Cationic π -Cyclization of an Isomuenchnone Derivative for the Synthesis of (\pm)-Lycopodine
- L4 ANSWER 19 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of optically active 2-cyclopentenone derivatives as anticancer agents for promotion of bone formation
- L4 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of β -lactone derivatives as anticholesteremics
- L4 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of trisubstituted benzene compounds for treating congestive heart failure
- L4 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI 1,3-Benzodithiolium cation mediated cyclization reactions
- L4 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Synthetic routes to the piperolides, fadyenolides, epoxypiperolides, and related compounds
- L4 ANSWER 24 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Search for new calcium antagonists. Lipophilic oximes and phosphonates
- L4 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Syntheses of the (\pm) -[n]-gingerols (pungent principles of ginger) and related compounds through regionselective aldol condensations: relative pungency assays
- L4 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI 2,3-Dihydropyrans
- L4 ANSWER 27 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Synthesis of (\pm) -[6]-gingerol (pungent principle of ginger) and relatives via directed aldol reactions

=> d 14 21 ti fbib abs

- L4 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of trisubstituted benzene compounds for treating congestive heart failure
- AN 1991:185027 CAPLUS
- DN 114:185027
- TI Preparation of trisubstituted benzene compounds for treating congestive heart failure
- IN Hawkins, Lynn D.
- PA Warner-Lambert Co., USA
- SO U.S., 15 pp. Cont. of U.S. Ser. No. 38,252, abandoned. CODEN: USXXAM
- DT Patent
- LA English
- FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI	US 4971959	Α	19901120	US 1988-292580	19881230
				US 1987-38252	19870414
	US 5274002	Α	19931228	US 1990-578965	19900906
				US 1987-38252	19870414
				US 1988-292580	19881230
OS ·	MARPAT 114:185027				

GI MARPAT 114:18502

AB The title compds. [I; R1 = C3-6 cycloalkyl; R2 = alkyl; X = O, S; A = bond, C1-7 alkylene, C2-6 alkenylene optionally interrupted by O, S, and imino; Y = CONR3R4 wherein R3, R4 = H, alkyl, azido, cyano] are prepared Hydrogenation of II [R = (E)-CH:CHCO2Me] (preparation given) over 5% Pd-C gave 83.9% propionate II (R = CH2CH2CO2Me), which was heated in anhydrous methanolic NH3 at 100° to give 32.0% I (R1 = cyclopentyl, R2X = MeO, A = CH2CH2, Y = CONH2) (III). III showed EC50 of 1 + 10-5M in improving coronary blood flow and increased heart contractility at 1.0 mg/kg in dogs.

=> logoff hold		7
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	7.72	164.61
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.70	-0.70

SESSION WILL BE HELD FOR 60 MINUTES
'STN INTERNATIONAL SESSION SUSPENDED AT 08:27:06 ON 06 OCT 2004

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * SESSION RESUMED IN FILE 'CAPLUS' AT 08:39:08 ON 06 OCT 2004 FILE 'CAPLUS' ENTERED AT 08:39:08 ON 06 OCT 2004 COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	7.72	164.61
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION

=> d his

(FILE 'HOME' ENTERED AT 08:22:00 ON 06 OCT 2004)

FILE 'REGISTRY' ENTERED AT 08:22:16 ON 06 OCT 2004

L1 STRUCTURE UPLOADED

L2 0 SEARCH L1 SSS SAM

L3 8 SEARCH L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:24:42 ON 06 OCT 2004
L4 27 L3

=> d 14 1-17 ti

L4 ANSWER 1 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN

- TI Fresh organically grown ginger (Zingiber officinale): composition and effects on LPS-induced PGE2 production
- L4 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of arylquinazolines and related derivatives for promoting the release of parathyroid hormone
- L4 ANSWER 3 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Use of a secondary or tertiary phenylated amines to smooth wrinkles
- L4 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Synthesis of polysubstituted furans by 2palladium-catalyzed coupling of butatrienyl carbinols with aryl halides and triflates
- L4 ANSWER 5 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Synthesis of N,N',N''-trisubstituted thiourea derivatives and their antagonist effect on the vanilloid receptor
- L4 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Synthesis and anticancer activity of nordihydroguaiaretic acid (NDGA) and analogues
- L4 ANSWER 7 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Process for producing cinnamyl aldehyde derivatives and use thereof as intermediate for aspartame derivative
- L4 ANSWER 8 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- ${\tt TI}$ N-Alkylaspartyl dipeptide esters and low-calorie sweeteners containing them
- L4 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI High hypolipidemic activity of saturated side-chain α -asarone analogs
- L4 ANSWER 10 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of $\beta\text{-alanine}$ derivatives as fibrinogen receptor antagonists
- L4 ANSWER 11 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Structural effects on the OH--promoted fragmentation of methoxy-substituted 1-arylalkanol radical cations in aqueous solution: the role of oxygen acidity
- L4 ANSWER 12 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Process for the production of aspartyldipeptide ester derivatives, novel intermediates therefor and process for the production of the intermediates

- ANSWER 13 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- A Novel Straightforward Synthesis of Enantiopure Tetrahydroisoquinoline TIAlkaloids
- ANSWER 14 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN T.4
- TIThe Synthesis and Evaluation of a Solution Phase Indexed Combinatorial Library of Non-Natural Polyenes for Reversal of P-Glycoprotein Mediated Multidrug Resistance
- L4ANSWER 15 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- Potent and Selective Non-Peptidic Inhibitors of Endothelin-Converting TI Enzyme-1 with Sustained Duration of Action
- L4ANSWER 16 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- ΤI Preparation of 1,4-dihydropyridine derivatives as antagonists against tolerance to anticancer drugs or potentiators for anticancer drugs
- L4ANSWER 17 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- A practical iodination of aromatic compounds using tetrabutylammonium ΤI peroxydisulfate and iodine

=> d 14 7 ti fbib abs

- L4ANSWER 7 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
- ΤI Process for producing cinnamyl aldehyde derivatives and use thereof as intermediate for aspartame derivative
- 2001:851092 CAPLUS AN
- DN 135:371997
- Process for producing cinnamyl aldehyde derivatives and use thereof as ΤI intermediate for aspartame derivative
- Mori, Kenichi; Fujita, Shinji; Funakoshi, Nao; Takemoto, Tadashi IN
- PAAjinomoto Co., Inc., Japan
- SO PCT Int. Appl., 29 pp. CODEN: PIXXD2
- DTPatent
- LAJapanese 1

FAN.CNT 1

	PATENT NO.				KIND		DATE		APPLICATION NO.									
ΡI	WO 2001087813					20011122		WO 2001-JP3545				20010424						
	W	: AE	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
			CR,															
	•		HU,															
			LU,															
		RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	
		VN,	YU,	ZA,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM				
	R	W: GH	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,	
		DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,	
		BJ	CF,	CG,	CI,	CM,	GA,	GN;	GW,	ML,	MR,	NE,	SN,	TD,	TG			
										JP 2	-000	1428	11	i	A 2	0000	516	
	EP 1283197		A1 20030212			EP 2001-922073				20010424								
•	R	: AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
		IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	ΑL,	TR							
										JP 2	-000	1428	11	Ž	A 2	0000	516	
										WO 2	001-	JP35	45	1	w 2	0010	424	
	US 2003163004			A1 20030828			US 2002-295997					2	0021	118				
										JP 2	-000	1428	11	i	A 2	0000	516	
									,	WO 2	001-	JP35	45	Ĭ	A1 2	0010	424	
OS	CASRE	ACT 13	35:37	1997	; MA	RPAT	135	:3719	997									

$$\begin{array}{c|c} & & & & \\ & & & \\ N & & & \\ N & & \\ N & & \\ \hline \\ N & & \\ CO_2Me \end{array}$$

AB Described is an industrial process for conveniently and efficiently producing highly pure cinnamyl aldehyde derivs. (I; R = H, C1-4 alkyl or alkoxy) such as (2E)-(3-hydroxy-4-methoxy)cinnamyl aldehyde which comprises reacting a benzaldehyde derivative (II; R = same as above) (for example, isovanillin) with acetaldehyde in the presence of an alkali, preferably adding acetaldehyde in portions in an aqueous solution at a low temperature

The cinnamyl aldehyde derivs. (I) thus obtained are selectively reduced into 3-(3-hydroxy-4-substituted phenyl)propionaldehydes (III; R = same as above). These compds. III are further subjected to reductive alkylation with aspartame to efficiently give N-[N-[3-(3-hydroxy-4-substituted phenyl)propyl]-L-α-aspartyl]-L-phenylalanine 1-Me esters (IV; R = H, C1-4 alkyl or alkoxy), which are useful as sweeteners with high sweetness. Thus, 121.72 g isovanillin and 320 g NaOH were dissolved in 2,000 mL H2O and cooled to -10°, followed by continuously adding 290 g 28 weight% aqueous acetaldehyde over a period of 45 h, and the resulting mixture was stirred for 1 h, treated with 768.1 g 36 weight% aqueous HCl, and filtered to give 324 g crystalline product. The latter product was dispersed in 500 mL H2O at 25°, treated with 97.5 g 25 weight% aqueous NaOH for dissoln., stirred with 4 g activated charcoal and 16 g celite, and filtered. The filtrate was neutralized with 55.4 g 36 weight% aqueous HCl to give 185.5 g crystalline product

IV

which was vacuum-dried, dispersed in 275 mL MeOH at 60°, stirred for 2 h, cooled to room temperature, and filtered to give, after drying the wet crystals, 83.2 g (2E)-3-hydroxy-4-methoxycinnamaldehyde (98% purity) in 57% yield. The latter compound (5.00 g) and 300 mg 5% Pd-Al2O3 were added to 80 mL MeOH and stirred under H atmospheric at 35° for 24 h, followed by filtration for removal of the catalyst and washing the catalyst with 10 mL MeOH, to give a MeOH solution of 3-(3-hydroxy-4-methoxyphenyl)propionaldehyde (87% yield). The latter solution (8.15 g) containing 1.50 g of the aldehyde

2.57 g aspartame were added to a 4:1 mixture of MeOH and H2O, followed by adding 0.7 g 10% Pd-C containing 50% H2O, and the resulting mixture was stirred at 35° under H atmospheric for 48 h to give 71% N-[N-[3-(3-hydroxy-4-methoxyphenyl)propyl]-L- α -aspartyl]-L-phenylalanine 1-Me ester.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

and

- TI High hypolipidemic activity of saturated side-chain α -asarone analogs
- AN 2001:830461 CAPLUS
- DN 136:128585

12:1

- TI High hypolipidemic activity of saturated side-chain α -asarone analogs
- AU Cruz, Adriana; Garduno, Leticia; Salazar, Maria; Martinez, Elizdath; Diaz, Francisco; Chamorro, German; Tamariz, Joaquin
- CS Departamento de Quimica Organica, Escuela Nacional de Ciencias Biologicas, IPN. Prol. Carpio y Plan de Ayala, Mexico, 11340, Mex.
- SO Medicinal Chemistry Research (2001), 10(9), 587-595 CODEN: MCREEB; ISSN: 1054-2523
- PB Birkhaeuser Boston
- DT Journal
- LA English
- AB With the aim of evaluating the pharmacophore potential of the side chain of α -asarone regarding its high hypolipidemic activity, α -asarone analogs (I) were evaluated pharmacol. For I, with a variable-size side chain, significant decreases in serum cholesterol, LDL-cholesterol, and triglyceride levels and significant increases in HDL-cholesterol levels were observed in mice. I were even more active than α -asarone in reducing cholesterol. The results suggested that the length and saturated character of the side chain seem to be a key feature in improving hypolipidemic activity of I.
- RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> logoff hold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
•	ENTRY	SESSION
FULL ESTIMATED COST	21.17	178.06
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.10	-2.10

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 08:43:20 ON 06 OCT 2004